Downloaded from orbit.dtu.dk on: May 05, 2023

DTU Library

A Thermodynamic Library for Simulation and Optimization of Dynamic Processes

Ritschel, Tobias Kasper Skovborg; Gaspar, Jozsef; Jørgensen, John Bagterp

Published in:
IFAC-PapersOnLine

Link to article, DOI:
10.1016/j.ifacol.2017.08.951

Publication date:
2017

Document Version
Publisher's PDF, also known as Version of record

Link back to DTU Orbit

Citation (APA):
Ritschel, T. K. S., Gaspar, J., & Jørgensen, J. B. (2017). A Thermodynamic Library for Simulation and Optimization of Dynamic Processes. *IFAC-PapersOnLine*, *50*(1), 3542-3547. https://doi.org/10.1016/j.ifacol.2017.08.951

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Available online at www.sciencedirect.com

ScienceDirect

IFAC Papers Online CONFERENCE PAPER ARCHIVE

IFAC PapersOnLine 50-1 (2017) 3542–3547

A Thermodynamic Library for Simulation and Optimization of Dynamic Processes ⋆

Tobias K. S. Ritschel, Jozsef Gaspar, John Bagterp Jørgensen

Department of Applied Mathematics and Computer Science & Center for Energy Resources Engineering (CERE), Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

Abstract: Process system tools, such as simulation and optimization of dynamic systems, are widely used in the process industries for development of operational strategies and control for process systems. These tools rely on thermodynamic models and many thermodynamic models have been developed for different compounds and mixtures. However, rigorous thermodynamic models are generally computationally intensive and not available as open-source libraries for process simulation and optimization. In this paper, we describe the application of a novel open-source rigorous thermodynamic library, ThermoLib, which is designed for dynamic simulation and optimization of vapor-liquid processes. ThermoLib is implemented in Matlab and C and uses cubic equations of state to compute vapor and liquid phase thermodynamic properties. The novelty of ThermoLib is that it provides analytical first and second order derivatives. These derivatives are needed for efficient dynamic simulation and optimization. The analytical derivatives improve the computational performance by a factor between 12 and 35 as compared to finite difference approximations. We present two examples that use ThermoLib routines in their implementations: (1) simulation of a vapor-compression cycle, and (2) optimal control of an isoenergetic-isochoric flash separation process. The ThermoLib software used in this paper is distributed as open-source software at www.psetools.org.

© 2017, IFAC (International Federation of Automatic Control) Hosting by Elsevier Ltd. All rights reserved.

Keywords: Thermodynamic library, Process simulation, Dynamic optimization, Vapor compression cycle, Vapor-liquid equilibrium, Flash separation

1. INTRODUCTION

Rigorous thermodynamic computations of vapor and liquid properties (volume, enthalpy, entropy) constitute a significant part of the computations in the dynamic simulation and optimization of many industrial processes governed by vapor-liquid equilibrium. Such processes are ubiquitous and include power cycles, vapor compression cycles, refrigeration systems, vapor-liquid separations in tanks, distillation columns, and oil reservoirs modeled by compositional and thermal models. Thermodynamic models, such as equations of state (EOS) and activity coefficient models, are widely used in the process industries and represent a certain level of complexity. As process simulation and optimization software depends critically on thermodynamic property computations, it is crucial to the computational performance that such thermodynamic models are implemented efficiently. Simulation and gradient-based optimization of dynamic process systems governed by vapor-liquid equilibrium require in addition to the thermodynamic properties themselves also first and in many cases second order derivatives of the thermodynamic properties.

In this paper, we present a performance study of a recently developed open-source thermodynamic library, ThermoLib, which is designed for efficient dynamic simulation and optimization. It is implemented in Matlab and C. The novelty of ThermoLib is that it provides routines for evaluating analytical first and second order derivatives with respect to temperature, pressure, and mole numbers. The derivatives are obtained with symbolic differentiation. The library is based on parameters and correlations from the DIPPR database (Thomson, 1996), the Peng-Robinson (PR) EOS (Peng and Robinson, 1976), the Soave-Redlich-Kwong (SRK) EOS (Soave, 1972), and the van der Waals mixing rules (Shibata and Sandler, 1989). ThermoLib is an open-source library and is available from www.psetools.org (Ritschel et al., 2016). There are already a few open-source libraries such as the simulink toolbox T-MATS by Chapman et al. (2014) and a Matlab library by Martín et al. (2011). Furthermore, the CALPHAD software OpenCalphad developed by Sundman et al. (2015) contains an open-source module for evaluation of thermodynamic properties. However, none of these libraries provide both first and second order derivatives.

We present two examples that use ThermoLib routines in their implementations, namely simulation of a heat pump and dynamic optimization of an isoenergetic-isochoric flash separation process. Heat pumps are promising for the recovery of waste and ground heat and have numerous complex applications in heating and cooling, i.e. air

⋆ This project is funded partly by: 1) Innovation Fund Denmark in the CITIES project (1305-00027B) and in the OPTION project (63-2013-3), 2) the interreg project Smart Cities Accelerator (10606 SCA), and 3) EUDP 64013-0558 in the IEA Annex for energy efficient process control.

2405-8963 © 2017, IFAC (International Federation of Automatic Control) Hosting by Elsevier Ltd. All rights reserved.
Peer review under responsibility of International Federation of Automatic Control.
10.1016/j.ifacol.2017.08.951

conditioning, floor heating, cryogenic air distillation, drying processes, etc. The European Heat Pump Association (2015) has reported that a total heat pump capacity of approximately 6.6 GW was installed in Europe during 2014, producing 13 TWh of energy and reducing CO_2-equivalent emissions by 2.09 Mt. Consequently, efficient simulation of heat pump devices is important to the design of economically attractive control methodologies, and will contribute to energy savings in both household and industrial applications. In the second example, we consider separation of hydrogen sulfide (H_2S) from a gas condensate. This is an example of a multi-component vapor-liquid equilibrium process that appears in e.g. distillation columns and is ubiquitous in the oil and chemical process industries.

This paper is structured as follows. Section 2 gives a brief description of the ThermoLib interface and presents a set of performance tests of selected library routines. Section 3 presents simulations of the heat pump and Section 4 presents an optimal control strategy for the flash separation process. Conclusions are given in Section 5.

2. THERMODYNAMIC LIBRARY

This section briefly discusses the interfaces of the ThermoLib Matlab routines that are used in the heat pump simulations presented in Section 3 and the optimal flash separation presented in Section 4. Furthermore, we present a set of performance tests that illustrate the efficiency of selected library routines. ThermoLib is open-source software available at www.psetools.org and its methods are described by Ritschel et al. (2016).

2.1 ThermoLib Matlab Interface

Fig 1(a) shows a Matlab script that computes molar vapor and liquid enthalpy, entropy, and volume of Freon-12 which is one of the refrigerants that are used in the heat pump simulations. The thermodynamic properties are evaluated at a temperature of $T = 300$ K and a pressure of $P = 1$ MPa. The Thermolib routine LoadParams must be called before using any other routine. It loads DIPPR parameters and in this case also PR EOS parameters. The two routines PureRealVapHSV and PureRealLiqHSV return the thermodynamic properties together with first and second order temperature and pressure derivatives. Fig. 1(b) shows a Matlab script that computes enthalpy, entropy and volume of a hydrocarbon mixture. ThermoLib requires that the user specifies a set of binary interaction parameters, k_{ij}. These are all zero for hydrocarbons. The properties are evaluated at a temperature of $T = 300$ K and a pressure of $P = 10$ MPa. The two routines MixRealVapHSV and MixRealLiqHSV return the thermodynamic properties, vectors of first order derivatives, and matrices of second order derivatives.

2.2 Computational Performance of ThermoLib

Fig. 2 shows a set of performance tests that evaluate eight of the main routines in ThermoLib. The routines compute vapor and liquid properties of real and ideal mixtures as well as of pure components. Fig. 2(a) compares the efficiency of the library routines to numerical differentiation. The mixture routines are between 12 and 35 times faster than numerical differentiation, while the pure component routines are around 5 times faster. The speedup is lower for the pure component routines because they only evaluate temperature and pressure derivatives. Fig. 2(b) shows the computation time of the Matlab, C and Mex routines. The C routines are more than a hundred times faster than the Matlab routines and around ten times faster than the Mex routines. The order of magnitude ranges from milliseconds for the Matlab routines to microseconds for the C routines. Fig. 2(c) and 2(d) show the increase in computation time for the Matlab and C routines with respect to the number of components. There is hardly any increase for the Matlab routines, which is due to efficient vectorization, while the increase is close to linear for the C routines.

3. VAPOR-COMPRESSION CYCLE

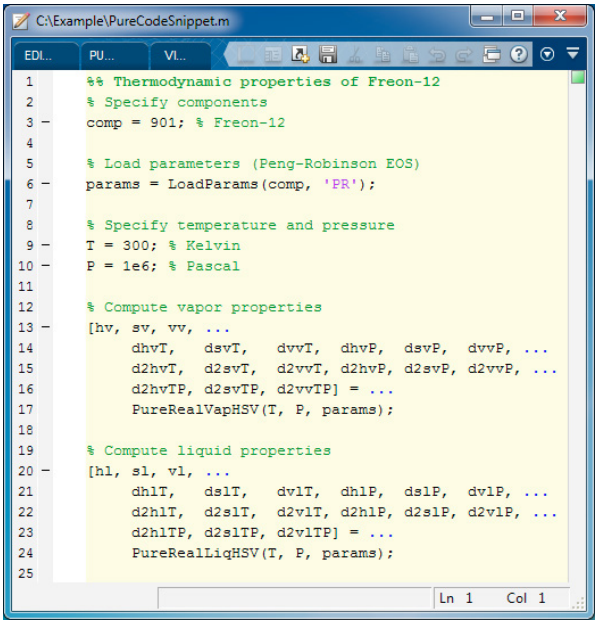
In this section we describe a vapor-compression cycle (VCC) for the modeling of heat pumps or refrigerators. Furthermore, we present the effect of ambient conditions on the performance of a heat pump in order to emphasize the need for thermodynamically rigorous computation of the efficiency of heat pumps.

A heat pump is a reversed heat engine that transfers heat from a low temperature zone to one with a higher temperature using mechanical work for compression. Fig. 3 shows a schematic drawing of a VCC with a typical temperature-entropy diagram. The VCC consists of four steps. First the low pressure and low temperature refrigerant (point 1) is evaporated in a heat exchanger producing a saturated vapor (point 2). This saturated low pressure vapor is compressed isentropically by supplying work, W_c, in the compressor to produce a high temperature and high pressure vapor (point 3). Afterwards, heat is released in the condenser at constant pressure, producing a saturated liquid phase (point 4). Finally, the saturated liquid is expanded to its original pressure at isenthalpic conditions in a turbine or in a throttling valve (point 1). The coefficient of performance (COP) provides the overall energy efficiency of a VCC used for either heating, $\mathrm{COP}_{\mathrm{heat}}$, or cooling, $\mathrm{COP}_{\mathrm{cool}}$. These COPs are defined as

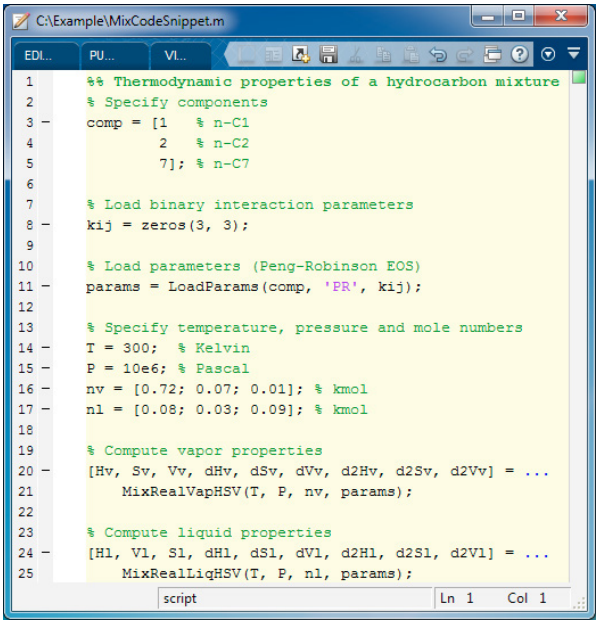
$$\mathrm{COP}_{\mathrm{heat}} = \frac{h_3 - h_4}{h_3 - h_2}, \tag{1a}$$

$$\mathrm{COP}_{\mathrm{cool}} = \frac{h_2 - h_1}{h_3 - h_2}, \tag{1b}$$

where h_1, h_2, h_3, and h_4 are the enthalpies of the refrigerant in the four points in the cycle. At nominal operating conditions, a COP of a heat pump is often set to 3. This indicates that the extracted heat is 3 times the energy input to the compressor. However, the COP is a nonlinear function of the evaporation temperature, condensation temperature, the active load, and the isentropic efficiency of the compressor. Therefore, thermodynamically correct and accurate modeling of this unit is necessary for reliably determining the performance of a VCC and for realistic optimal control of processes with integrated heat pumps. The dynamics of VCCs are in general much faster than the dynamics of buildings and industrial processes (Halvgaard et al., 2012; Hovgaard et al., 2013; Jensen and Skogestad, 2007; Svensson, 1996; Zhao et al., 2003). Therefore, we implement a static model of a heat pump. This model is based



(a) Computation of thermodynamic properties of Freon-12.



(b) Computation of thermodynamic properties of a hydrocarbon mixture.

Fig. 1. Examples of Matlab scripts that use ThermoLib routines to compute thermodynamic properties.

on energy conservation equations, and ThermoLib routines are used for the computation of enthalpy, entropy, and saturation pressure as well as their temperature and pressure derivatives. Fig. 4 shows the solution methodology that is used to compute the COP of this static VCC model. For a single component refrigerant, this implementation relies on the ThermoLib routines `PureRealVapHSV` and `PureRealLiqHSV`, whose interfaces were briefly presented in Section 2, and the `PureRealSatTemp` routine.

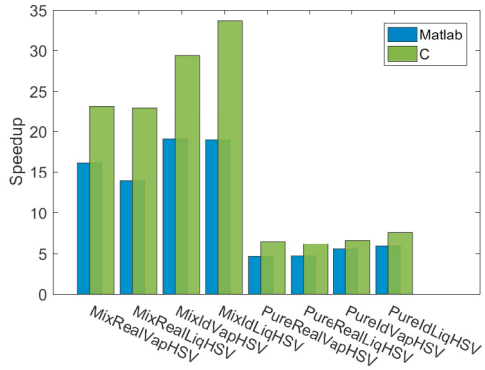
3.1 Simulation Results

This section presents simulations of two frequently encountered operational scenarios and it illustrates that the efficiency of a heat pump is strongly dependent on ambient conditions and the type of the refrigerant.

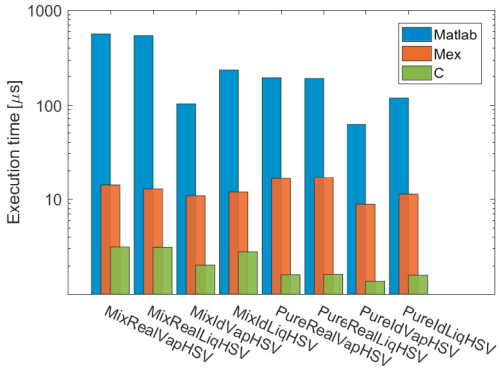
Fig. 5 shows the simulation results for Freon-12 and CO_2. Fig. 5(a) shows the effect of changes in the evaporation temperature on the performance (COP) of a heat pump. The condenser operates at a fixed 20°C. This scenario frequently occurs in the case of heat pumps for indoor climate control aiming at maintaining a constant room temperature during daily and seasonal changes of the ground temperature. Fig. 5(b) shows the COP as function of the condensation temperature at a fixed evaporation temperature of −10°C. This scenario occurs when heat pumps absorb energy from a constant heat source while the released heat is a manipulated variable. Such scenarios are encountered in many industrial applications, for instance in cryogenic air distillation. The results shown in Fig. 5 illustrate that the COP is significantly affected by changes in the operation parameters and that it also depends on the type of refrigerant. Consequently, the assumption of a constant COP, often used in control applications, is not realistic. Realistic simulations and conclusions require a rigorous thermodynamic library such as ThermoLib.

4. FLASH SEPARATION PROCESS

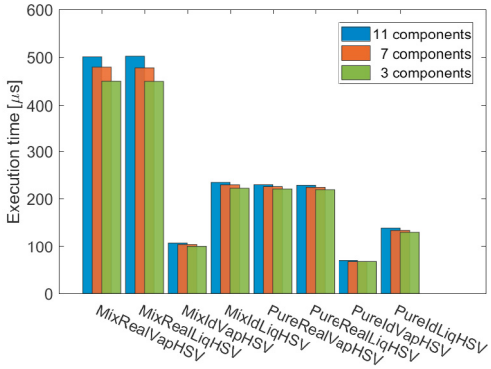
In this section, we present an optimal control strategy for a flash separation process in which H_2S is removed from a gas condensate. The condensate consists of eleven hydrocarbons as well as CO_2, N_2, and H_2S. The separation process is assumed to be at vapor-liquid equilibrium. The dynamic optimization of the isoenergetic-isochoric (UV) flash process can be formulated as a bilevel optimization problem (Ritschel et al., 2017). The inner optimization problem is the 2nd law of thermodynamics that says that equilibrium of a closed systems is obtained at maximum entropy of the system. The outer dynamic optimization problem has the differential mass and energy balances in addition to the equilibrium conditions as constraints. The mass and energy balances are affected by a feed stream that supplies the gas condensate to the separator unit, a vapor stream that extracts gas, a liquid stream that extracts liquid, and a heat input. The separator unit is sketched in Fig. 6. We apply a model-based approach to find an optimal control strategy with respect to a given performance measure, while satisfying a set of constraints. We use a single shooting approach which combines dynamic simulation with an iterative optimization algorithm (Binder et al., 2001). Fig. 7 illustrates the solution methodology. Model-based control is advantageous because it can be used for both setpoint tracking and economical control, and because it can handle constraints. However, it is also computationally expensive and therefore it is important to accelerate the computations by applying a gradient-based optimization method. This requires the first and second order derivatives of thermodynamic properties because the first order derivatives appear in the vapor-liquid equilibrium conditions in the model. They are provided by ThermoLib. The gradients of input bound constraints are derived analytically while output bound constraints are incorporated into the objective function using a logarithmic



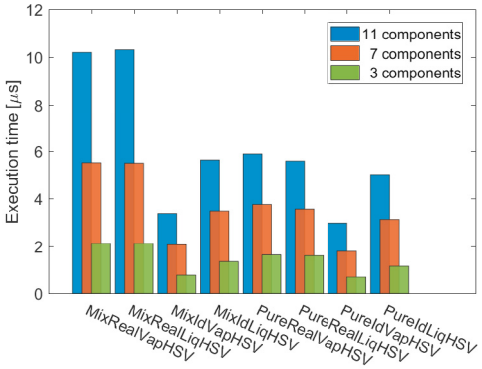
(a) Speedup in computation time compared to numerical forward difference approximations of first and second order derivatives for benzene, toluene and diphenyl.



(b) Computation times of the Matlab, C and Mex routines. Pure component routines evaluate benzene properties and mixture routines evaluate properties of a mixture of benzene, toluene and diphenyl.



(c) Computation times of the Matlab routines for 3 components: n-C_1 to n-C_3, 7 components: n-C_1 to n-C_7, and 11 components: n-C_1 to n-C_{11}.



(d) Computation times of the C routines for 3 components: n-C_1 to n-C_3, 7 components: n-C_1 to n-C_7, and 11 components: n-C_1 to n-C_{11}.

Fig. 2. Performance tests of eight Matlab, C, and Mex routines from ThermoLib. The functionality is related to the routine names as follows. Mix: mixture properties, Pure: pure component properties, Real: real properties, Id: ideal properties, Vap: vapor properties and Liq: liquid properties.

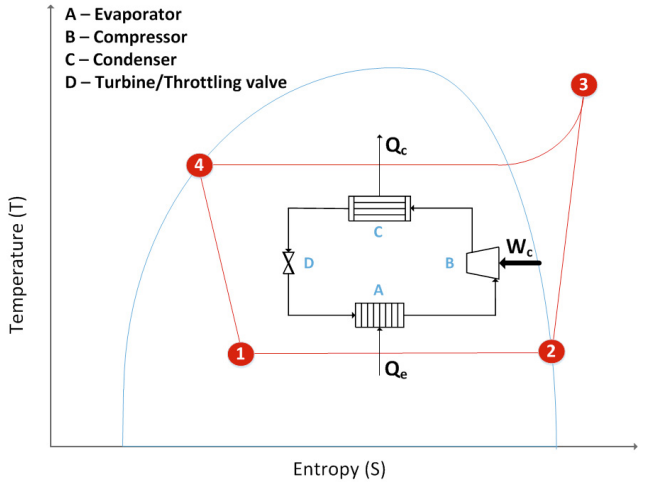


Fig. 3. Schematic representation and temperature-entropy diagram of a vapor-compression cycle.

barrier function. An adjoint method is used for computing the gradients of the objective function (Jørgensen, 2007).

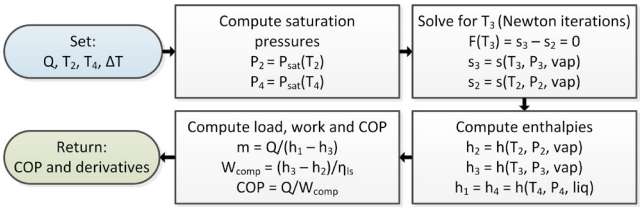
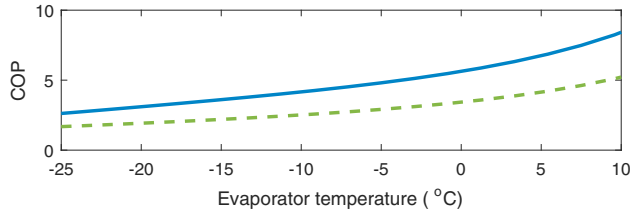


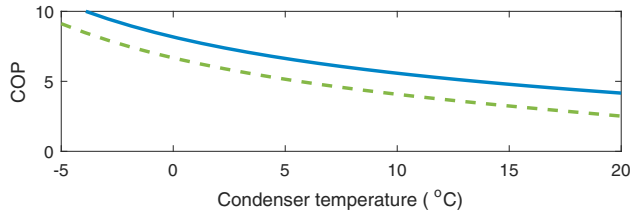
Fig. 4. Solution methodology for simulation of the static model of the vapor-compression cycle. T_1 through T_4 are temperatures, and P_1 through P_4 are pressures.

4.1 Optimal Control Example

We present an example where the gas condensate is processed over a time interval of six hours, i.e. $t \in [t_0,\ t_f] = [0\text{ hr},\ 6\text{ hr}]$. During the middle two hours the H_2S content of the feed increases significantly as shown in Fig. 8(a). The manipulated variables are the vapor stream flow rate, F_V, and the heat input, Q. We consider the heat input to be a cooling device such that $Q \leq 0$. The objective is to minimize the amount of energy spent on cooling, i.e. to maximize the functional



(a) COP as function of evaporation temperature.



(b) COP as function of condensation temperature.

Fig. 5. Heat pump simulations of common operational scenarios. Blue solid: Freon-12. Green dashed: CO_2.

$$\phi = \int_{t_0}^{t_f} Q(t)dt \tag{2}$$

subject to the following constraint on the H_2S vapor mole fraction, y_{H_2S}

$$y_{H_2S}(t) \leq y_{H_2S}^{\max}, \qquad t \in [t_0, t_f], \tag{3}$$

where $y_{H_2S}^{\max} = 0.02$ is an upper bound on the level of impurity of the gas condensate. The liquid stream flow rate is controlled such that the total mass is constant, i.e. $F_L = F_F - F_V$ where $F_F = 12$ kmol/hr is the feed flow rate. We compare the optimal strategy with a reference strategy, which also satisfies the constraint (3). The vapor mole fraction of H_2S is shown in Fig. 8(a), and Fig. 8(b) shows the optimal control strategy (solid blue) and the reference strategy (green dashed). The optimal control solution only applies cooling during the step in the H_2S feed content where it is used to ensure that the constraint (3) is satisfied. The optimal strategy makes active use of the vapor flow rate. However, it processes the same amount of gas as the reference strategy. The energy spent on cooling is decreased from 600 MJ for the reference strategy to 370 MJ for the optimal strategy. This is an improvement of 38%. The single-shooting method requires 165 dynamic simulations to converge to the optimal control strategy shown in Fig. 8(b). The dynamic simulations are the main computational part of the single shooting approach. If the gradients of the objective function were approximated with finite differences it would not be necessary to compute second order derivatives of the thermodynamic properties. However, that would require at least 19,724 dynamic simulations. This is nearly 120 times as many simulations and it is likely that the computation time would increase by two orders of magnitude. This illustrates the potential of using the ThermoLib routines for efficient gradient-based solution of dynamic optimization problems.

5. CONCLUSIONS

We have presented a performance study of the recently developed thermodynamic library, ThermoLib, which is implemented in Matlab and C. The study shows that the computation time is of the order milliseconds for the Matlab routines and microseconds for the C routines.

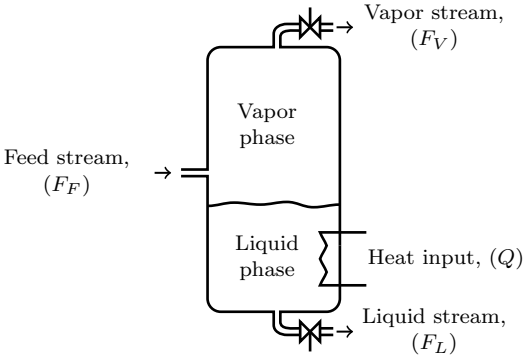


Fig. 6. Sketch of vapor-liquid flash separation unit.

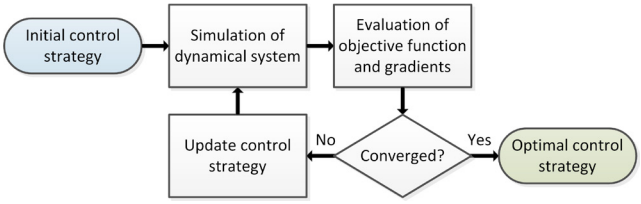


Fig. 7. Flow diagram of a gradient-based single shooting approach for dynamic optimization.

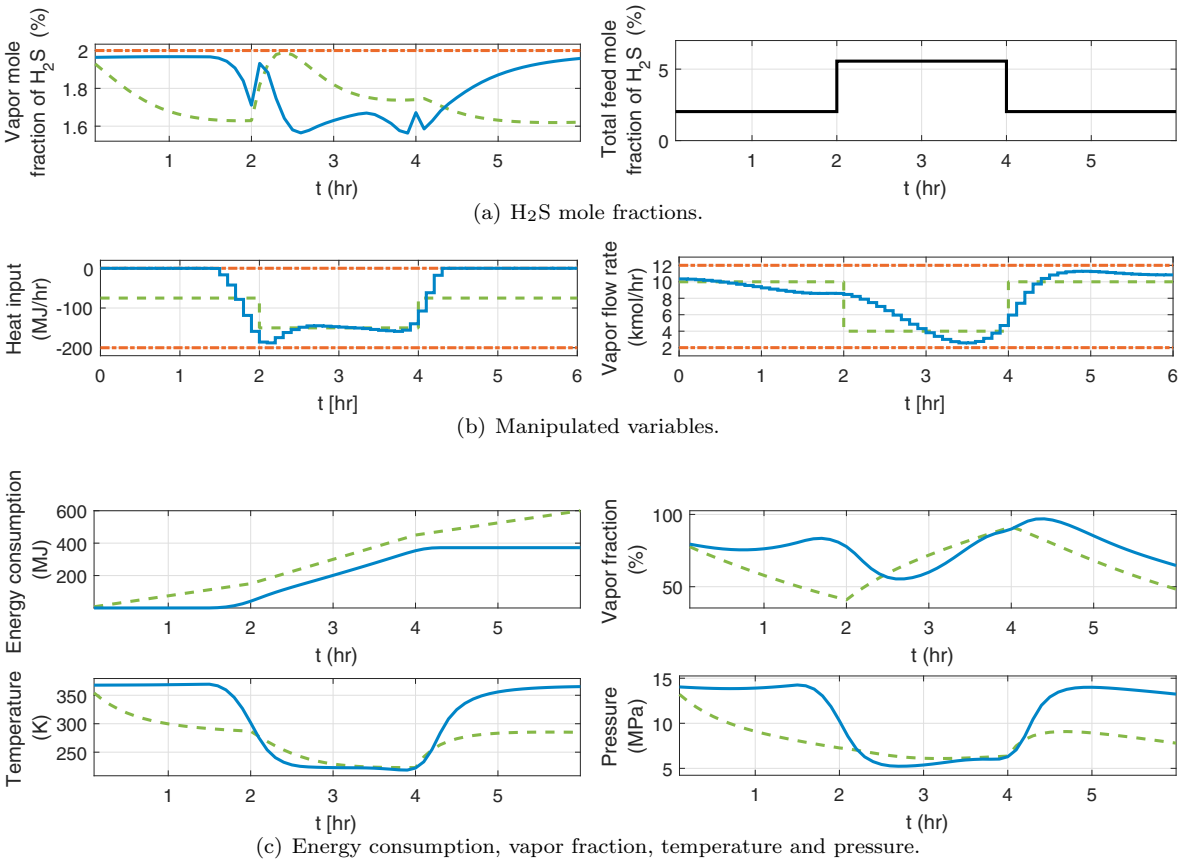
ThermoLib routines evaluate first and second order derivatives analytically which is an order of magnitude faster than numerical differentiation for mixture properties and around 5 times faster for pure component properties. The computation time is nearly constant with respect to the number of components for the Matlab routines and close to linear for the C routines.

Furthermore, we have used ThermoLib in the simulation of a vapor-compression cycle and for optimal control of a flash separation process. The study of the vapor-compression cycle outlined the importance of a rigorous thermodynamic approach for reliable predictions of process performance and economics with respect to different operating conditions and different types of refrigerants. The study demonstrated that assuming a constant coefficient of performance for a compression cycle, as is generally considered in control studies, may lead to significant prediction errors. Furthermore, we have solved a dynamic optimization problem involving a flash process using efficient gradient-based methods based on ThermoLib routines. The dynamic optimization problem involved nonlinear output constraints that were incorporated into the objective function using a barrier function, and the gradients of the objective were computed using an adjoint method. In both examples the availability of first and second order gradients is crucial to the good computational performance.

REFERENCES

Binder, T., Blank, L., Bock, H. G., Bulirsch, R., Dahmen, W., Diehl, M., Kronseder, T., Marquardt, W., Schlöder, J. P., von Stryk, O., 2001. Introduction to model based optimization of chemical processes on moving horizons. In: Online optimization of large scale systems. Springer, pp. 295–339.

Chapman, J. W., Lavelle, T. M., May, R. D., Litt, J. S., Guo, T.-H., 2014. Toolbox for the modeling and analy-



(a) H_2S mole fractions.

(b) Manipulated variables.

(c) Energy consumption, vapor fraction, temperature and pressure.

Fig. 8. Optimal flash separation of a gas condensate with a high content of H_2S. Blue solid: Optimal strategy. Green dashed: Reference strategy. Red dash-dotted: Bounds.

sis of thermodynamic systems (T-MATS) user's guide. Tech. rep., NASA's Glenn Research Center.

European Heat Pump Association, 2015. European heat pump market and statistics report 2015. Tech. rep., EHPA, Brussels.

Halvgaard, R., Poulsen, N. K., Madsen, H., Jørgensen, J. B., Jan 2012. Economic model predictive control for building climate control in a smart grid. In: 2012 IEEE PES Innovative Smart Grid Technologies (ISGT). pp. 1–6.

Hovgaard, T. G., Boyd, S., Larsen, L. F., Jørgensen, J. B., 2013. Nonconvex model predictive control for commercial refrigeration. International Journal of Control 86 (8), 1349–1366.

Jensen, J. B., Skogestad, S., 2007. Optimal operation of simple refrigeration cycles part ii: Selection of controlled variables. Computers and Chemical Engineering 31 (12), 1590–1601.

Jørgensen, J. B., 2007. Adjoint sensitivity results for predictive control, state- and parameter-estimation with nonlinear models. In: European Control Conference (ECC), 2007. pp. 3649–3656.

Martín, Á., Bermejo, M. D., Mato, F. A., Cocero, M. J., 2011. Teaching advanced equations of state in applied thermodynamics courses using open source programs. Education for Chemical Engineers 6 (4), e114–e121.

Peng, D.-Y., Robinson, D. B., 1976. A new two-constant equation of state. Industrial & Engineering Chemistry Fundamentals 15 (1), 59–64.

Ritschel, T. K. S., Capolei, A., Jørgensen, J. B., 2017. Dynamic optimization of UV flash processes. In: FOCAPO / CPC 2017.

Ritschel, T. K. S., Gaspar, J., Capolei, A., Jørgensen, J. B., 2016. An open-source thermodynamic software library. Tech. Rep. DTU Compute Technical Report-2016-12, Department of Applied Mathematics and Computer Science, Technical University of Denmark.

Shibata, S. K., Sandler, S. I., 1989. Critical evaluation of equation of state mixing rules for the prediction of high-pressure phase equilibria. Industrial & engineering chemistry research 28 (12), 1893–1898.

Soave, G., 1972. Equilibrium constants from a modified Redlich-Kwong equation of state. Chemical Engineering Science 27 (6), 1197–1203.

Sundman, B., Kattner, U. R., Palumbo, M., Fries, S. G., 2015. OpenCalphad - a free thermodynamic software. Integrating Materials and Manufacturing Innovation 4 (1).

Svensson, M. C., 1996. Model-based optimizing control of a water-to-water heat pump unit. Modeling, Identification and Control 17 (4), 279–295.

Thomson, G. H., 1996. The DIPPR® databases. International Journal of Thermophysics 17 (1), 223–232.

Zhao, L., Zhao, L. L., Zhang, Q., Ding, G. L., 2003. Theoretical and basic experimental analysis on load adjustment of geothermal heat pump systems. Energy Conversion and Management 44 (1), 1–9.